

Heisenberg antiferromagnet on Cayley trees: low-energy spectrum and even/odd site imbalance

Hitesh J. Changlani,¹ Shivam Ghosh,¹ Christopher L. Henley,¹ and Andreas M. Läuchli²

¹Laboratory of Atomic And Solid State Physics, Cornell University, Ithaca, NY 14853, USA

²Institut für Theoretische Physik, Universität Innsbruck, A-6020 Innsbruck, Austria

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To understand the role of local sublattice imbalance in low energy spectra of $s = \frac{1}{2}$ quantum antiferromagnets (as observed by [L. Wang and A.W. Sandvik, Phys. Rev. Lett. **97**, 117204 (2006); Phys. Rev. B **81**, 054417 (2010)]), we study the $s = \frac{1}{2}$ quantum nearest neighbor Heisenberg antiferromagnet on the coordination 3 Cayley tree. We perform many-body calculations using an implementation of the Density Matrix Renormalization Group (DMRG) technique for generic tree graphs. We discover that the bond-centered Cayley tree has a quasi-degenerate set of low lying tower of states and an “anomalous” singlet-triplet finite size gap scaling. For understanding the construction of the first excited state from the many-body ground state, we consider a wavefunction ansatz given by the single mode approximation (SMA), which yields a high overlap with the DMRG wavefunction. Observing the ground state entanglement spectrum helps us to analytically understand the scaling of the finite size spin gap and leads us to a picture of the low energy degrees of freedom being “giant spins” arising out of sublattice imbalance. The Schwinger Boson mean field theory has been generalized to *non uniform* lattices and ground states have been found which are spatially inhomogeneous in the mean field parameters.

I. INTRODUCTION

Quantum antiferromagnetism for unfrustrated systems has been one of the most extensively researched subjects in condensed matter physics. One of the simplest models in this family, the nearest neighbor spin $\frac{1}{2}$ Heisenberg antiferromagnet on the square lattice, has been studied extensively: analytically with Spin Wave¹⁻³ and Schwinger Boson approaches⁴⁻⁸ and numerically with Quantum Monte Carlo⁹(which has no “sign problem” for bipartite lattices). That said, effects from physical imperfections such as the presence of open edges^{10,11} and static non magnetic impurities¹² are less well understood and hence are areas of active research. Random dilution, for example, has been found to affect the low energy spectrum drastically, as has been demonstrated in recent numerical studies by Wang and Sandvik¹³. They showed that the singlet-triplet energy gap on finite clusters, at the percolation threshold, is much smaller than that expected from the conventional Anderson tower of states (or “quantum rotor” states)¹⁴⁻¹⁸. This was in disagreement with a previous theoretical result¹⁹.

Wang and Sandvik attributed the mechanism of the creation of this low energy scale to the presence of regions of “local sublattice imbalance”, arising out of areas in the cluster where the number of opposite sublattice sites were unequal. In their picture, geometric constraints of a diluted square lattice forbid spins from pairing up with their neighbors into dimers, leaving some of them unpaired or “dangling”¹³. They believe these emergent spins to be the effective low energy degrees of freedom.

By considering the undiluted nearest neighbor Heisenberg model on the Cayley tree (or Bethe Lattice) (shown in Fig. 1) we have been able to systematically investigate the effect of sublattice imbalance on the low energy spectrum. In particular, we contend that the effect of sublattice imbalance is to create a “tower of states”, lower than the Anderson tower of states. Aided by numerical calculations, we propose a framework for understanding this relationship. We also find that Schwinger Boson Mean Field theory⁵ is a good description

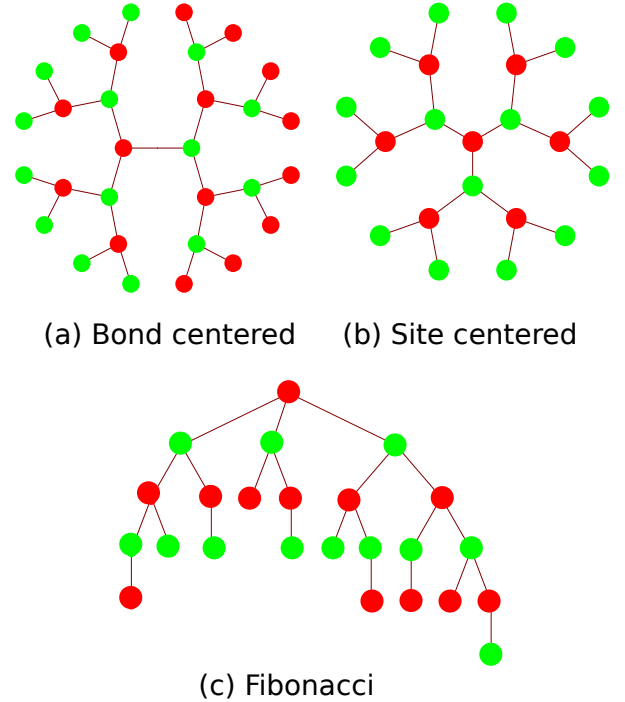


Figure 1: (Color online) (a) The bond-centered Cayley tree. (b) The site-centered Cayley tree. In both cases all sites, other than those on the boundary, have coordination 3. (c) The “Fibonacci Cayley tree” is constructed hierarchically and has some coordination 2 sites. Our choice is motivated by the fact that such a cluster has no local sublattice imbalance (refer text for details). All clusters are bipartite (the dark(red) and light(green) colors show the two sublattices) and have no loops.

of the many body ground state and can reproduce many of its features quantitatively.

Previous studies of this model by Otsuka²⁰ and Friedman²¹ focussed primarily on ground state properties and excited

states were not considered in these studies. More recently Kumar et. al²² have significantly extended this analysis to both the spin-1/2 and spin-1 Heisenberg model. We use all these studies as useful benchmarks for our own numerical calculations.

The Cayley tree is a lattice without loops, with all sites (except those on the boundary) having a coordination z . The number of sites on the boundary is asymptotically the same as the number of sites in the bulk. This is a pathology of the Cayley tree, in contrast to lattices in Euclidean space. As a consequence, different ways of approaching the thermodynamic limit may give different results in any problem based on the Cayley tree. In particular, when we use three different limiting sequences of finite clusters (see sec. II), we find qualitatively different limiting behaviors; a central thrust of the paper is to explain why. But it is generally possible in Cayley tree problems to define a “bulk” limit if, rather than averaging expectations over the entire cluster, one evaluates them only within a cluster of some fixed size which is kept at the center while the boundaries get farther and farther away.

In the literature, the “Bethe lattice” is often used to refer to the thermodynamic limit of the “Cayley tree”, where the effect of boundaries is eliminated (see for example Laumann et.al²³ which considers random graphs of fixed connectivity). For the purpose of this paper, the presence of open boundaries will play an important role in the low energy physics and so we will simply use the term “Cayley tree” from now on.

From a theorist’s perspective, the Cayley tree achieves many simplifications which makes exact solutions possible. For example, the Bose Hubbard model on this lattice has been recently solved by Semerijan, Tazria and Zamponi²⁴. It has also been used as a tool to study the Brinkman-Rice transition for the Hubbard model²⁵. It has also found applications in the treatment of the quantum impurity problem which is at the heart of Dynamical Mean Field Theory (DMFT)²⁶. There has also been interest in the study of dendrimers^{27–29}, but it does not appear that a spin model has been realized on such a topology experimentally.

The complete absence of loops makes this lattice conducive for the Density Matrix Renormalization Group (DMRG) algorithm³⁰. With the DMRG method we have an explicit (yet compact) representation of ground and excited state many body wavefunctions which gives us lots of information to understand the low energy properties of these systems. In particular, reduced density matrices can be used as tools to understand properties of these states³¹.

Various versions of the DMRG have been used^{20–22} to study the spin 1/2 Heisenberg model on the Cayley tree. In addition, Lepetit et. al³², have considered the fermionic Hubbard model at half filling. More recently, Murg et. al³³ have also used the Cayley tree to embed quantum chemical systems to study them with tree tensor network algorithms (closely related to the DMRG).

The remainder of the paper is divided as follows. In section II we introduce the model and lattices being investigated and define a measure of sublattice imbalance associated with them. In section III, we give a brief overview of our implementation of the DMRG algorithm applied to generic trees.

In section IV, we discuss the general properties of the ground state and excited states of the bond-centered Cayley tree. In section V, we use a variational ansatz given by the single mode approximation, in conjunction with an argument from first order perturbation theory, to explain the finite size scaling of the spin gap. Finally, in section VI, we corroborate our observations of the ground state properties, by the use of the Schwinger Boson mean field theory (SBMFT).

II. THE MODEL

We consider the nearest neighbor antiferromagnetic spin 1/2 Heisenberg model with uniform coupling J ,

$$H = J \sum_{\langle i,j \rangle} \vec{s}_i \cdot \vec{s}_j \quad (2.1)$$

In this paper, we use spin rotational symmetry of the Hamiltonian (2.1), to label many body states by $|S, S_z\rangle$, where S refers to the spin of the state and S_z is its z component.

On a bipartite lattice (with sublattices A and B), like the Cayley tree, with n_A sites in sublattice A and n_B sites in sublattice B , it is rigorously known³⁴ that the ground state of the Heisenberg Hamiltonian has a net spin $S = \left\lfloor \frac{n_A - n_B}{2} \right\rfloor$.

The first kind of tree we consider is the “bond-centered” Cayley tree of the form depicted in Fig. 1(a). The number of sites N_s for such a cluster is related to the “generation” g by,

$$N_s(g) = 2^{g+1} - 2 \quad (2.2)$$

Since the bond centered clusters have no “global imbalance” i.e. $n_A = n_B$, the ground state is a singlet. We have observed that the first excited state is a triplet.

As mentioned before, the notion of “local sublattice imbalance” will be crucial in understanding the low energy physics. For the bond centered cluster, we define a measure of imbalance (which we refer to as I_b from here on) by dividing the cluster at the central bond into two equal parts. We count the excess of one sublattice over the other in one half of the cluster and multiply by 1/2 for spin 1/2. It can be easily shown that $I_b(g)$ is related to the generation g as,

$$I_b(g) = \frac{2^g \pm 1}{6} \quad (2.3)$$

where $+$ ($-$) is for g odd(even).

Fig. 1(b) is the more usual way of defining a Cayley tree and which we refer to as “site-centered”. The number of sites is related to the generation g by,

$$N_s(g) = 3(2^g - 1) + 1 \quad (2.4)$$

Unlike the bond centered cluster, a global sublattice imbalance exists here which leads to a ground state spin of $S_0 \equiv 2^{g-1}$. We find it convenient to measure the imbalance $I_s(g)$ in either of the three symmetrical arms of the site centered Cayley tree. As before, we measure the excess sites of one sublattice over the other (in one arm) and multiply by 1/2. This definition is particularly convenient as it gives us $I_s(g) = I_b(g)$ for all g .

A recent publication on the study of the Heisenberg model on the Cayley tree by Kumar, Ramasesha and Soos²² considers the site-centered clusters. We confirm their results for the site-centered case, but interestingly find that the bond-centered cluster has significantly different ground and excited state properties. We will provide some brief comparisons in section IV to illustrate this point.

How is the situation different if there is no imbalance locally? To address this, we introduce the "Fibonacci Cayley tree", an example of which is shown in Fig. 1(c). The recipe for generating this lattice is to make generation $g + 1$ by attaching one branch each from generation g and $g - 1$. If we label the number of odd/even sublattice sites by A_g and B_g , then (counting the root as even), we get,

$$A_{g+1} = 1 + B_g + B_{g-1} \quad (2.5a)$$

$$B_{g+1} = A_g + A_{g-1} \quad (2.5b)$$

The total number of sites N_s at generation $g + 1$ is,

$$N_s(g + 1) = A_g + B_g = 1 + N_s(g) + N_s(g - 1) \quad (2.6)$$

Observe that $N_s(g)$ satisfies the Fibonacci recursion (hence the name). The size of this lattice grows as τ^g where τ is the golden ratio $\tau = (1 + \sqrt{5})/2 \sim 1.618$. Also, every 3rd generation is unbalanced by 1 (and every other generation is both globally and locally balanced).

In order to have a balanced cluster at every generation, we combine two identical generation g Fibonacci constructions (as in equation (2.6)), by introducing a bond connecting their roots.

III. DENSITY MATRIX RENORMALIZATION GROUP ON GENERIC TREE GRAPHS

The Density Matrix Renormalization Group (DMRG) is a powerful numerical technique for studying many-body systems. It was developed by White³⁰ for one dimensional systems to remedy the problems associated with the Numerical Renormalization Group (NRG)³⁵. Otsuka²⁰ and B. Friedman²¹ realized that the DMRG is also applicable to the Cayley tree. Their procedure was for regular trees and utilized an infinite-system DMRG. A recent publication by Kumar et. al²² (for the site-centered lattice) improves upon the scaling of previous algorithms, by considering an efficient way to hierarchically construct the lattice.

Our implementation differs from all of the above, as it allows us to study the properties of *any* finite tree (and not necessarily regular ones, eg. percolation clusters³⁶). We outline the details in the remainder of this section.

We spell out the notation we have used in this section. d is the number of degrees of freedom per site. For example, $d = 2$ for a spin 1/2 Hamiltonian. z is the coordination number of a site (Although our discussion talks in terms of uniform z , a generalization to site dependent z is straightforward). M will be used to denote the number of retained states on a local cluster of sites (or "block").

A. Initialization

Our algorithm starts with the generation of a suitable guess wavefunction. As Fig. 2 shows, this is done by performing energy based truncations of the Hilbert space on a successive hierarchy of clusters of sites (or "blocks"), assuming they are completely disconnected from the rest of the system. By "energy based truncation" we mean that on each block we retain only the M lowest energy states of the local block Hamiltonian, where M is a parameter that determines the accuracy of the calculation. This procedure is carried out in parallel, beginning from the boundary sites of the cluster and terminating when one reaches the geometrically central point (called the "focal" point or "root").

While the end result of our calculations are expected to be independent of this initialization, a good choice can greatly accelerate convergence. In addition, when targeting an excited state (say in a high S_z sector), we often introduce a "fake" magnetic field in the Hamiltonian to favor retention of those states on the blocks that describe the high energy wavefunction.

At the end of the initialization calculation, one has a crude description of the full Hamiltonian in terms of the root degree of freedom surrounded by z blocks.

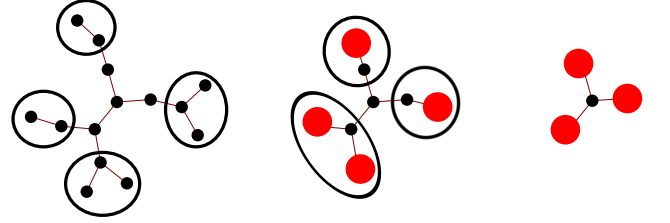


Figure 2: Warm-up step of the DMRG involving multiple independent renormalization procedures on the tree utilizing energy based truncation. The "army continues to march in" from all sides till one reaches the geometrically central point (often called the "focal point" or "root"). Here we show all stages for a given tree. The red dots represent renormalized blocks.

B. Density matrix based truncation

We will now consider how every "iteration" in the DMRG is carried out to systematically approach the ground (or excited) state(s) of the system. For this purpose, we require a description of the full Hamiltonian in terms of a "site" degree of freedom (here (\uparrow, \downarrow)) and the basis spanned by the M^z states retained on the z blocks surrounding it.

At every iteration we use the Lanczos algorithm³⁷ to solve for the lowest energy eigenvector. Treating one of the blocks as the "environment" and the remaining $z - 1$ blocks and the "site" collectively as the "system", we obtain the reduced density matrix (RDM) of the system from the ground state of the superblock by computing;

$$\rho_{RDM} \equiv \text{Tr}_{\text{env}} (|\psi_{\text{GS}}\rangle \langle \psi_{\text{GS}}|) \quad (3.1)$$

Each block takes its turn being the "environment" while the other blocks together with the "site" act as the system. (The order of choosing environments is not very crucial to the final result.)

In addition to the ground state density matrix, we have also targeted higher excited states, by performing a state averaging of the reduced density matrix,

$$\rho_{RDM}^{avg} \equiv \frac{\sum_i w_i \text{Tr}_{\text{env}} (|\psi_i\rangle\langle\psi_i|)}{\sum_i w_i} \quad (3.2)$$

where w_i is the positive weight given to the density matrix formed from state $|\psi_i\rangle$. In most cases, we simply used $w_i = 1$ for all states we targeted. An advantage of state averaging is that it often helps us to prevent (or get us out of) solutions which are local (but not global) minima. The reduced density matrix is diagonalized and only M states with the highest eigenvalues (out of the total dM^z states) are kept on the block.

C. Sweep algorithm

The root of the tree has no special significance in the algorithm once the initial guess wavefunction has been created and a representation of the block states has been generated. For example, once the density matrix based truncations with the root as "site" are completed, the algorithm proceeds to consider a new division of the lattice into "systems" and "environment" by considering a site on the shell one step out from the root. Each of the z sites connected to the original root gets its turn being the "new root".

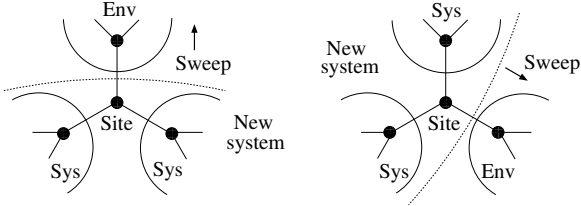


Figure 3: Division of the Cayley tree locally into site, system(s) and environment as required by the DMRG. One renormalization step consists of combining the site and system(s) into a new system, retaining the states governed by tracing out the environment degrees of freedom.

Once we reach the exterior of the cluster, we "sweep in". However, this time (and for all future sweeps) we have an environment present, whose states we trace over to guide the density matrix based truncation process. This in-out-in sweep continues till convergence of the energy is attained. Thus the scaling of algorithm is $zN_s m^{z-1}d$ where N_s is the number of sites in the tree. For a highly symmetrical lattice (such as the Cayley tree), one can reduce this computational cost to $z \log(N_s) M^{z-1}d$ (however this has not been implemented). One complete sweep is defined here as a sweep out (from the root to the boundaries) followed by a sweep in (from boundaries to the root) operation.

D. Computing Expectations

Just as in the usual one dimensional DMRG, we have an explicit representation of the wavefunction in terms of the block states and we can efficiently compute various kinds of correlation functions. For the purpose of this paper, we have simply measured the spin-spin correlation functions $\langle \vec{s}_i \cdot \vec{s}_j \rangle$ and the matrix element $\langle 1 | s_i^+ | 0 \rangle$, where $|0\rangle$ ($|1\rangle$) refers to the ground state singlet (first excited state triplet) and has the labels $|S=0, S_z=0\rangle$ ($|S=1, S_z=1\rangle$). Both these functions are needed for calculating the coefficients occurring in the single mode approximation, which will be discussed in section V. The latter is computed by targeting the ground and excited state in the same DMRG run, so that both states have the same block representation.

We also study the eigenvalues of the reduced density matrix (for a particular division of the lattice), collectively known as the "entanglement spectrum". These turn out to be a very useful probe of the low energy degrees of freedom (as we will see in section VC). This needs no extra effort in the DMRG, since these eigenvalues are computed anyway as part of the truncation process.

E. Parameters and Benchmarks

All calculations reported here are for the $z=3$ case and $M \leq 160$. For all systems considered here we get reasonable convergence of the energy within 20 sweeps.

To benchmark our calculations we have also compared our results with Exact Diagonalization data where possible. In particular, for the bond centered tree we considered the ground state energies and correlations in all S_z sectors of the 30 site cluster and some high S_z sectors for the 62 site cluster.

One can see from Table I that the convergence of the energy and the spin gap is rapid as a function of the number of retained states on a block (M) for the site centered (in the $S_z = S_0$ sector) and Fibonacci trees (in the $S_z = 0$ sector). However, for the bond centered case (Table II), the convergence with M is much slower. We observed that it was only towards the $M=100$ mark that the $SU(2)$ symmetry of the wavefunctions began to be restored in our calculation. While larger M calculations are certainly desirable, we believe the present calculations are reasonable and confirm the existence of an anomalous energy scale in the many body spectrum of the bond centered tree.

M	$N_s = 190$		$N_s = 176$	
	E_{GS}	Δ	E_{GS}	Δ
20	-74.54049387	0.9397293	-76.46983049	0.08834668
60	-74.54054021	0.9397198	-76.47071767	0.08725531
100	-74.54054022	0.9397198	-76.47072851	0.08725207

Table I: Energy (E_{GS}) and Spin gap (Δ) for the 190 site site-centered and 176 site Fibonacci lattices for various values of M .

The question of finite size scaling can be considered tricky given the small magnitude of the singlet-triplet gap. However, by computing the ground state energies in every S_z sector, and fitting the "tower of states", we believe the errors are mitigated.

M	E_{GS}	Δ	$\langle 1 s_c^+ 0 \rangle$	$\langle 1 s_b^+ 0 \rangle$
60	-49.3405119	3.4×10^{-4}	0.310	0.370
80	-49.3412938	5.7×10^{-4}	0.300	0.344
100	-49.3415002	6.0×10^{-4}	0.280	0.337
120	-49.3415347	6.0×10^{-4}	0.279	0.335
140	-49.3415521	6.0×10^{-4}	0.278	0.335

Table II: Energy (E_{GS}), Spin gap (Δ) and s^+ matrix elements for the central (c) and boundary (b) sites for the 126 site bond-centered for various values of M . $|0\rangle$ and $|1\rangle$ refer to the lowest singlet and triplet respectively.

IV. GROUND AND EXCITED STATES

Using the DMRG algorithm presented in section III, we calculate the ground state energy and spin gap, which serve to point out the differences between the bond and site centered clusters. To highlight the role of local imbalance, we also compare the excited states of the bond-centered and Fibonacci trees, both of which are globally balanced.

A. Ground State Energy, Spin-spin correlations and Spin Gap

We consider the bond-centered, site-centered and Fibonacci clusters and compute the ground state energy and the spin gap Δ defined as,

$$\Delta = E_{GS}(S_0 + 1) - E_{GS}(S_0) \quad (4.1)$$

where S_0 is the spin of the ground state.

In order to compute the energy per site in the infinite lattice limit e_0 we fit $\frac{E_{GS}}{N_s}$ to the functional form,

$$\frac{E_{GS}}{N_s} = e_0 + \frac{a}{N_s} + \frac{b}{N_s^2} \quad (4.2)$$

Depending on whether we fit the bond or site-centered clusters we get $e_0 = -0.393855(2)$ and $e_0 = -0.393854(2)$ respectively both of which are consistent within error bars of extrapolation and with the value of $e_0 = -0.39385$ reported by Ref. 22.

In comparison, as Table III shows, the energy per site of the Fibonacci tree is significantly lower than either of the bond or site centered trees. This is done by the formation of very strong nearest neighbor dimers (especially on the boundary as the degree of dimerization dies down as one proceeds inwards). The degree of boundary dimerization is more limited in the site and bond centered trees.

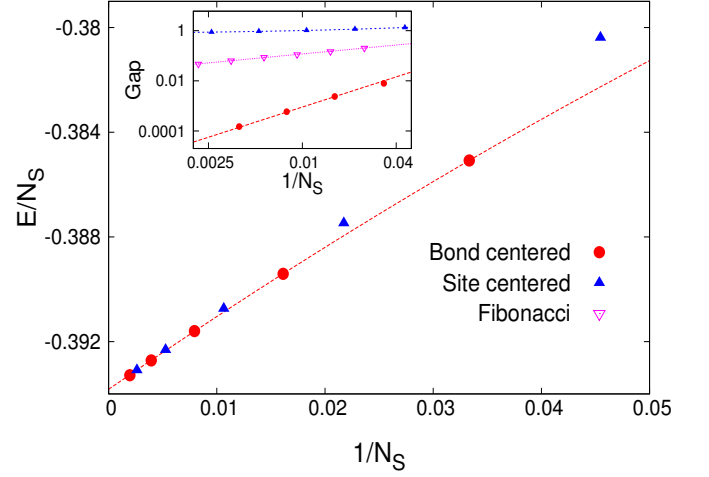


Figure 4: Ground state energy per site for the bond centered and site centered Cayley trees for various lattice sizes. The Fibonacci Cayley tree energies are out of the scale considered. A fit to the bond centered results given by Eq.(4.2) has been shown. Inset: Finite size scaling of the energy gap Δ plotted on a log-log scale. The bond-centered and Fibonacci clusters appear gapless in the infinite lattice limit, with a finite size scaling exponent of $\alpha \approx 2$ and $\alpha \approx 0.6$. However, the site-centered clusters have a finite Δ in the infinite lattice limit in concordance with the results of Ref. 22. The lines shown are fits to the DMRG data using equations(4.3, 4.4).

Despite the dissimilarities between the three lattices, the "bulk limit" of the estimated energy per bond, based on taking an average of nearest neighbor $\langle \vec{s}_i \cdot \vec{s}_j \rangle$ over the innermost bonds, is roughly identical for all three kinds of Cayley tree, about $-0.35J$.

Cluster	e_0	a	b	Δ
Bond centered	-0.393855(2)	0.292(1)	-1.05(4)	$\sim N_s^{-2}$
Site centered	-0.393854(1)	0.291(1)	+0.099(3)	$0.73 + 2.86/\sqrt{N_s}$
Fibonacci	-0.435433(1)	0.167(1)	-0.42(4)	$\sim N_s^{-0.6}$

Table III: Ground state energy per site e_0 , finite size scaling parameters for the ground state energy a, b (from Eq.(4.2)) and spin gap Δ (from equations(4.3,4.4) for the bond-centered, site-centered and Fibonacci clusters.

We now turn to a discussion of the spin gap. The site-centered cluster has a spin gap in the infinite lattice limit, which we obtained by fitting to,

$$\Delta = \Delta_\infty + \frac{c}{N_s^\alpha} \quad (4.3)$$

and found Δ_∞ to be 0.731(4) and $\alpha \sim 0.5$.

The bond-centered and Fibonacci clusters appear to be gapless in the infinite lattice limit, based on cluster sizes up to 254 and 464 sites respectively. We computed the finite size scaling of this gap using,

$$\Delta \sim N_s^{-\alpha} \quad (4.4)$$

Empirically, the value of $\alpha \sim 0.6$ for Fibonacci and $\alpha \sim 2$ for the bond centered clusters matches rather well with our data (see inset of Fig. 4).

Denoting the ground state as $|0\rangle$, we also compute the ground state connected correlation function defined here as,

$$G_{ij} \equiv \langle 0 | \vec{s}_i \cdot \vec{s}_j | 0 \rangle - \langle 0 | s_i^z | 0 \rangle \langle 0 | s_j^z | 0 \rangle \quad (4.5)$$

For the bond-centered and Fibonacci clusters, $\langle 0 | s_i^z | 0 \rangle = 0$ for all i , and hence we have,

$$G_{ij} = \langle 0 | \vec{s}_i \cdot \vec{s}_j | 0 \rangle \quad (4.6)$$

Fig. 5 shows some sample correlation functions on all three lattices. The marked difference in the behavior of the spin gap and the spin correlations between the site- and bond-centered clusters can be attributed to a different manifestation on the two type of clusters of the spontaneous spin symmetry breaking occurring in the thermodynamic limit. First, the behavior of the spin correlations can be understood in the following way: on the site centered clusters, the system has an extensive total spin $S = 2^{g-1}$ in the ground state. By choosing a particular state out of this large multiplet it is possible to orient the Néel vector at no energy cost in this finite size system. In particular if one considers the $S^z = S$ state of the multiplet, the local $\langle s_i^z \rangle$ expectation values will reflect the ordering pattern directly. This situation is somewhat analogous to ferrimagnetic systems. In the case of the bond-centered clusters we have a unique $S = 0$ ground state, which forbids finite $\langle s_i^z \rangle$ expectation values on a finite system, and the long-range order then has to be coded in the correlation functions leveling off to a finite value at long distances.

B. Low energy Tower of States

For the balanced Heisenberg antiferromagnet ($n_A = n_B$ with a singlet ground state) on a regular unfrustrated lattice (e.g. square in 2D or cubic in 3D), with number of sites N_s , it has been noted and argued^{17,18} that the low energy Hamiltonian can be described by a rigid rotor model,

$$H_{rot} = \frac{\vec{S}^2}{2I} = \frac{S(S+1)}{2I} \quad (4.7)$$

where \vec{S} is the total angular momentum (spin), and

$$I \cong \chi N_s \quad (4.8)$$

where χ is the susceptibility of \vec{S} to a field coupling to it. Thus, we have a sequence of multiplets, popularly referred to as the "Anderson Tower of States", which become degenerate in the limit $N_s \rightarrow \infty$ thus making $SU(2)$ symmetry breaking possible in this limit.

To see if this behavior is found on the Cayley tree, we computed the ground state energy in every S_z sector. This may be identified with the multiplet energy $E(S)$, since $E(S)$ is monotonic in S and $S \geq S_z$.

For the bond centered clusters, a tower of states exists, but an anomalous one. In Fig. 6 we observe that in the bond-centered case, the $E(S)$ curve consists of *two* linear pieces,

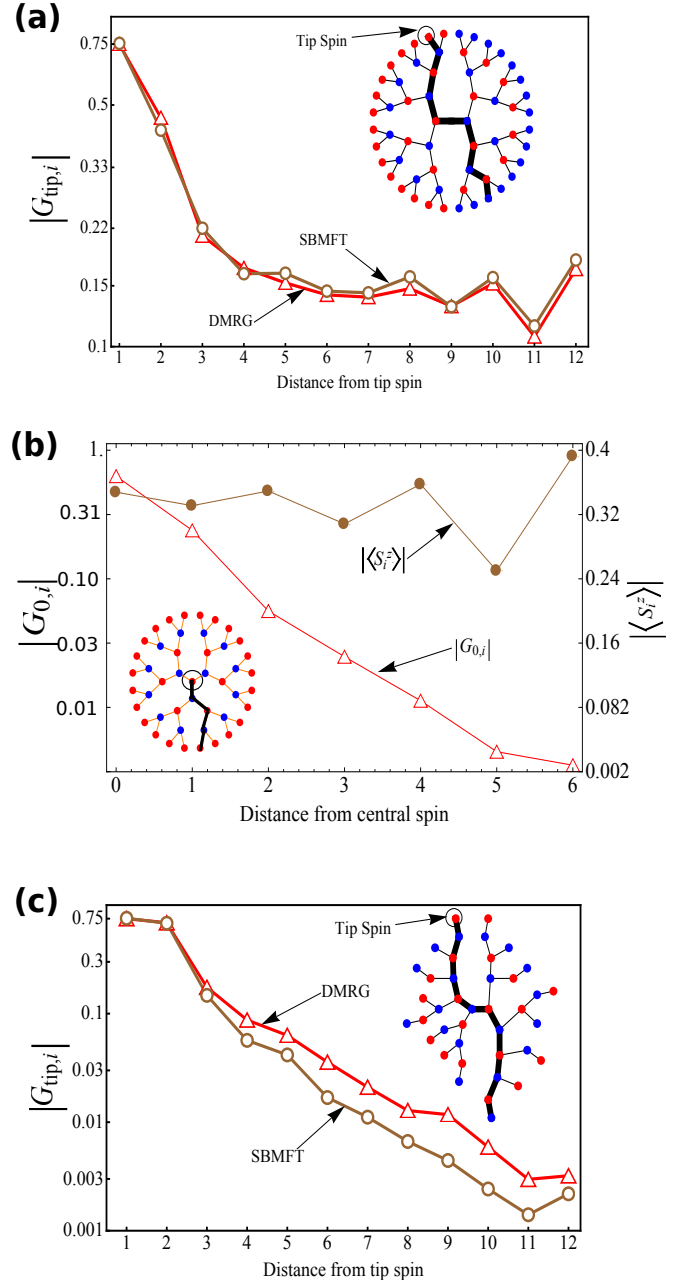


Figure 5: (Color online) Ground state spin-spin correlations $G_{a,i}$, as in equation (4.5), for the three kinds of Cayley tree. One (reference) spin a is held fixed while the other spin i is taken at distance a along the highlighted path. In (a) and (c), the reference spin is at a tip ($a \rightarrow \text{tip}$), and DMRG results are compared with numerical solutions of Schwinger Boson mean field theory (SBMFT) from Section VI. In (b), the reference spin is at the central ("root") site ($a \rightarrow 0$). (a) Bond-centered tree with $N_s = 126$ sites. The SBMFT correlations shown have been scaled up by an overall factor of 1.8 to take into account corrections beyond mean field (in the broken symmetry phase). The DMRG and SBMFT results show good agreement, asymptoting to a constant. (b) Site-centered cluster with $N_s = 190$ sites, in the maximum S_z member of the ground state multiplet ($S_z = S_0$). The magnetization $|\langle s_i^z \rangle|$ is also shown, as a function of distance from the center. Even though the connected correlation function decays to zero exponentially fast, the long range order is encoded in the fact that the magnetization is non zero. (c) Fibonacci tree with $N_s = 40$ sites. For the "quantum disordered" phase, the SBMFT correlations were scaled up by an overall factor of 3/2 (For details see sec. VIB). Correlations appear to be decaying exponentially with distance.

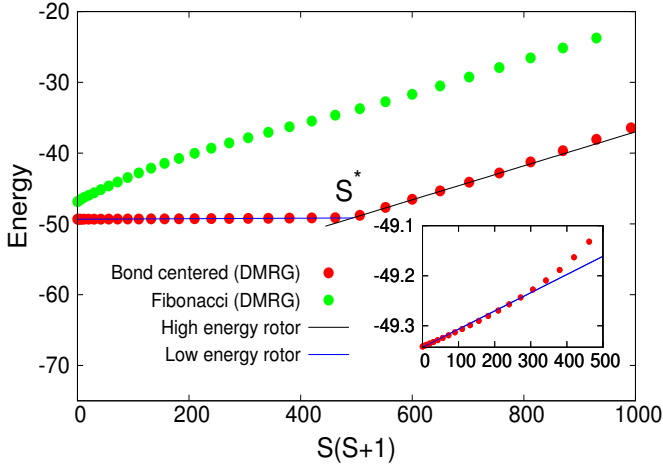


Figure 6: Lowest energy level in every S_z sector for the 108 Fibonacci and the 126 site bond-centered Cayley tree. The range of S from 0 to S^* has been magnified and shown in the inset for the 126 site cluster. It shows a tower of states with a much larger moment of inertia than expected from the Anderson tower. This is seen as a sharp kink like feature at S^* . In contrast, for the Fibonacci tree, the transition from the low to high S behavior is less well defined.

joined at a critical spin S^* which depends on the cluster size. In effect, the system has two moments of inertia, I_{low} for $S < S^*$ and the (much smaller) I_{high} for $S > S^*$. Fig. 7 plots the size dependence of these moments of inertia, showing that $I_{\text{low}} \sim N_s^2$ while $I_{\text{high}} \sim N_s$; it will be our task in Sec. V C, to explain this difference. We also observe that

$$S^* = 2I_b \quad (4.9)$$

where I_b is the sublattice imbalance on one half of the bond-centered cluster as defined in equation (2.3).

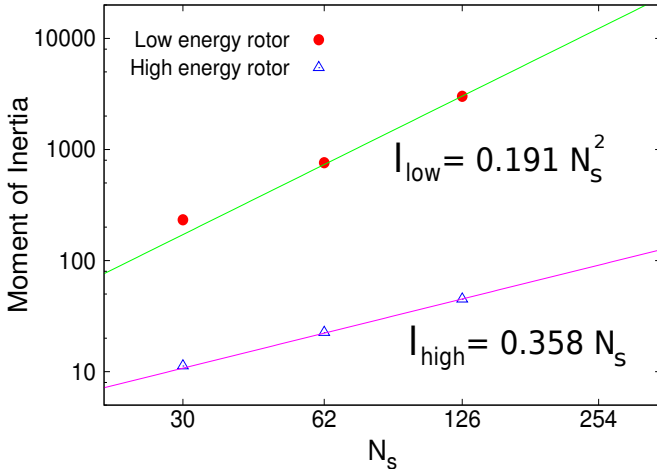


Figure 7: Moment of inertia of the low (I_{low}) and high energy (I_{high}) rotors as a function of lattice size (N_s) for the bond centered tree of various sizes as shown on a log-log plot.

For the Fibonacci tree, we do not find a clear distinction between the two linear pieces as seen in Fig. 6. The scaling of

the energy gaps ($E(S+1) - E(S)$) changes from $N_s^{-0.6}$ for small S , to $1/N_s$ Anderson scaling for large S (4.7).

In contrast with the gapless spectrum of the bond-centered and Fibonacci clusters, the site-centered case has a finite spin gap (see Table III) in the infinite lattice limit.

A complementary probe of the low energy physics is the magnetization (m) (see Fig. 8) defined as,

$$m = \frac{1}{N_s} \sum_i \langle s_i^z \rangle_{GS} \quad (4.10)$$

as a function of a uniform applied magnetic field h . We observe a rapid increase in magnetization for small h and it seems the saturation magnetization is about $m^* \sim 1/6$ (i.e. $m^*/m_{\text{sat}} \sim 1/3$). Beyond this rapid rise of the magnetization at small field, the magnetization curve displays a surprisingly rich structure, with several plateau-like features at intermediate magnetization, linked by more susceptible parts of the magnetization curve. We note that the first plateau at m^* seems to have a similar extent in magnetic field as for the site-centered clusters studied in Ref. 22. The detailed characterization of the magnetization curve as $N_s \rightarrow \infty$ appears to be an interesting problem for future studies.

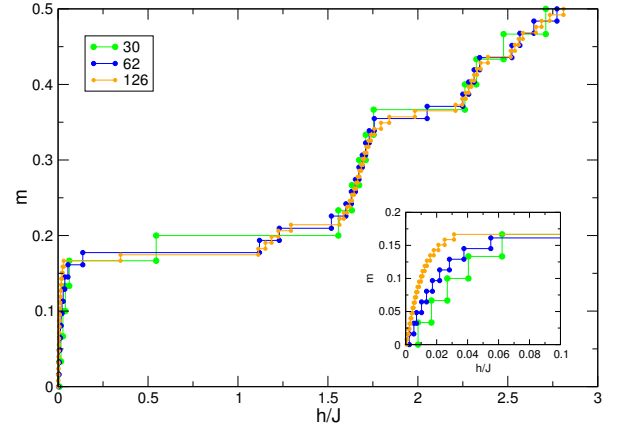


Figure 8: Magnetization curves for bond-centered Cayley trees of various sizes obtained using DMRG. Inset: The rapid rise of the magnetization with application of a small magnetic field indicates a susceptibility diverging with system size.

V. SINGLE MODE APPROXIMATION FOR THE EXCITED STATE

Can we understand the origin of these "anomalous" states within a unified framework for treating sublattice imbalance? In order to answer this, we study the nature of the triplet excited state and its relation to the ground state using the single mode approximation³⁸ (SMA for short). Assuming the knowledge of the ground state wavefunction $|0\rangle$ (analytically or from a numerical method), the SMA ansatz for the trial

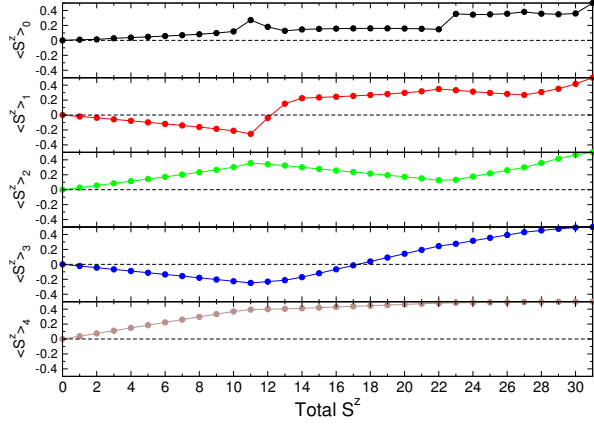


Figure 9: Magnetization curves for sites on various shells on the 62 site bond-centered Cayley tree. The subscript refers to the shell on which the site is present, that is, 0 refers to the central two sites and the 4 refers to the boundary. The boundary spins have a high local susceptibility.

state $|1'\rangle \equiv |S = 1, S_z = 1\rangle$ state is given by,

$$|1'\rangle = \frac{1}{\mathcal{N}_{1'}} \sum_{j=1}^{N_s} u_j s_j^+ |0\rangle \quad (5.1)$$

where u_j are variational parameters and $\mathcal{N}_{1'}$ is a normalization factor given by,

$$\mathcal{N}_{1'} \equiv \sqrt{\sum_{k,l} u_k^* u_l \langle 0 | s_k^- s_l^+ | 0 \rangle} \quad (5.2)$$

Using the spin symmetry of the Hamiltonian (and hence its eigenfunctions) and the fact that the ground state has $S_z = 0$, the normalization factor $\mathcal{N}_{1'}$ (5.2) can be written as,

$$\mathcal{N}_{1'} = \sqrt{\sum_{k,l} \frac{2}{3} u_k u_l G_{kl}} \quad (5.3)$$

where G_{kl} is the spin-spin correlation function previously defined in Eq.(4.6).

For a singlet ground state, observe that, there is a gauge degree of freedom in the choice of the SMA wavefunction (5.1), an arbitrary constant shift u , i.e.,

$$\sum_i u_i s_i^+ |0\rangle = \sum_i (u_i + u) s_i^+ |0\rangle \quad (5.4)$$

since for a ground state with total spin $S = 0$,

$$u \sum_i s_i^+ |0\rangle = u S_{tot}^+ |0\rangle = 0 \quad (5.5)$$

It can also be shown⁵¹ that the normalization $\mathcal{N}_{1'}$ in Eq.(5.3) is invariant under the transformation $u_i \rightarrow u_i + u$.

For a given trial state ψ_T which is a function of some parameters u_j , the variational principle guarantees that,

$$E_T \equiv \frac{\langle \psi_T(\{u_j\}) | H | \psi_T(\{u_j\}) \rangle}{\langle \psi_T(\{u_j\}) | \psi_T(\{u_j\}) \rangle} \quad (5.6)$$

where E_0 refers to the energy of the lowest lying state with the same symmetry as the trial wavefunction. The best wavefunction is obtained by optimization of the parameters \bar{p} by minimizing the variational energy E_T . Note that within the SMA formalism, the ground state (and hence the ground state energy) is assumed, which implies that the SMA spin gap is also a variational estimate for the true spin gap.

Here we will show that the SMA does turn out to be a very good ansatz for this system based on the close to 100 % overlap of the SMA wavefunction with the wavefunction from DMRG. Our procedure does not require explicit knowledge of the wavefunction, rather only certain matrix elements and correlation functions are necessary. Taking intuition from numerical calculations, we construct coefficients u_j occurring in Eq.(5.1) to obtain a simple variational state with a gap that goes to 0 faster than $1/N_s$. The aim of this section is thus to understand the operator that creates the triplet wavefunction from the ground state singlet. This in turn will tell us how the spins collectively act, accurately predicting the existence of an "anomalous" energy scale.

A similar SMA calculation was performed by Laumann et. al³⁹, who considered AKLT models on the Cayley tree. Instead of making their assumption of exponentially decaying spin-spin correlations, we use the values of $\langle 1 | s_i^+ | 0 \rangle$ and G_{ij} from our DMRG calculations. In addition, we make no assumptions about the variational parameters $\{u_j\}$.

A. Obtaining the SMA coefficients from maximization of overlap with the true wavefunction

The overlap of an approximate wavefunction with the exact one can serve as a good measure of its quality. Thus we consider the overlap of the SMA wavefunction with the true triplet state $|1\rangle \equiv |S = 1, S_z = 1\rangle$ i.e.,

$$\begin{aligned} O &\equiv \langle 1 | 1' \rangle \\ &= \frac{\sum_j u_j f_j}{\sqrt{\sum_{k,l} \frac{2}{3} u_k u_l G_{kl}}} \end{aligned} \quad (5.7)$$

and try to maximize it. We have defined f_i to be,

$$f_i \equiv \langle 1 | s_i^+ | 0 \rangle \quad (5.8)$$

We christen this term the "flippability" of a spin. This is motivated from its very definition: the more easily flipped spins have a larger contribution to the formation of the first excited triplet.

Now we present a method to obtain the optimal parameters u_j to construct $|1'\rangle$. To meet the requirements of a high overlap of the SMA wavefunction $|1'\rangle$ with the exact many body triplet $|1\rangle$, subject to the constraint that it is normalized, we devise a cost function C_{SMA} defined as,

$$C_{SMA} = - \sum_j u_j f_j + \lambda (\mathcal{N}_{1'}^2 - 1) \quad (5.9)$$

where we have introduced λ as a Lagrange multiplier. Taking $\{u_j\}$ as our variational parameters, and setting the derivatives

of C_{SMA} to 0, we get,

$$\frac{\partial C_{SMA}}{\partial u_i} = -f_i + \frac{4}{3}\lambda \sum_{l \neq i} u_l G_{il} + \lambda u_i = 0 \quad (5.10)$$

Thus we get the set of equations (one equation for each i),

$$f_i = \frac{4}{3}\lambda \sum_j G_{ij} u_j \quad (5.11)$$

To explicitly obtain a state $|1'\rangle$ which has a high overlap with $|1\rangle$, we solve the above linear equations for u_i numerically. Note that the matrix G always has exactly one zero eigenvalue because of the gauge degree of freedom (5.4). Hence we can not simply invert G to obtain u_i . Instead of inverting G , we directly solve the linear system of equations (5.11) using dgesv in LAPACK.

A natural choice of gauge for the parameters $\{u_j\}$ is to satisfy,

$$\sum_i u_i = 0 \quad (5.12)$$

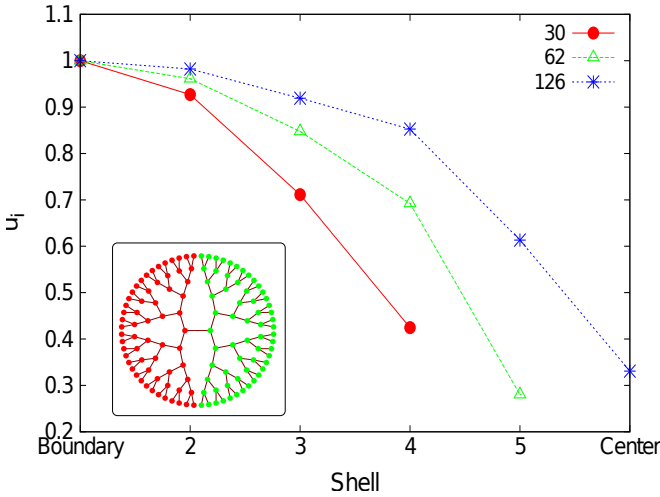


Figure 10: (Color online) Amplitude of the SMA coefficients u_i for various shells (normalized with respect to amplitude on the boundary) for the $N_s = 30, 62$ and 126 site bond-centered lattices. Inset: The sign structure of u_i is the same as equation (5.14). Dark(red) and light(green) indicates negative and positive u_i respectively.

Our observation from the numerical solution of equation (5.11) for the bond-centered Cayley tree is that $u_i > 0$ for i on one side of the central bond and $u_i < 0$ on the other side. We have also plotted the amplitudes of the optimal SMA coefficients for the 30, 62 and 126 site balanced Cayley trees in Fig. 10.

B. Comparison of various SMA wavefunctions

We next try to understand the qualitative nature of the SMA solution from the perspective of minimizing the triplet energy.

We consider various functional forms for u_i and numerically compute their overlap with the exact triplet and compare SMA gap estimates.

For the nearest neighbor Heisenberg model, the SMA gap is given by (for a derivation refer to Appendix A),

$$\Delta_{SMA} = \frac{-\sum_{\langle k,l \rangle} (u_k - u_l)^2 G_{kl}}{2 \sum_{ij} u_i u_j G_{ij}} \quad (5.13)$$

Observe that the numerator and denominator (being proportional to \mathcal{N}_1^2) are invariant under the transformation $u_i \rightarrow u_i + u$.

To minimize the SMA gap, one would like to minimize the numerator and maximize the denominator of equation (5.13) (note both the numerator and denominator are positive). To minimize the numerator, we can try to keep $u_k \approx u_l$ for as many bonds as possible, and hence consider the "left-right" ansatz,

$$u_i = \begin{cases} +1 & i \in \text{left of central bond} \\ -1 & i \in \text{right of central bond} \end{cases}$$

which is consistent with the gauge condition (5.12). This sign structure is in concordance with the numerical solution of equations (5.11) for the bond centered Cayley tree.

Note that this is quite contrary to the "staggered pattern", one obtains by solving equations (5.11) for the square lattice. The staggered pattern is defined as,

$$u_i = \begin{cases} +1 & i \in \text{even sublattice} \\ -1 & i \in \text{odd sublattice} \end{cases}$$

The staggered pattern is an energetically expensive solution for the bond-centered Cayley tree. Even though it maximizes the denominator making it $O(N_s^2)$, the numerator is also large i.e. $O(N_s)$. Thus the SMA gap scales only as $O(1/N_s)$.

Table IV verifies the arguments presented above by explicitly listing out the SMA gap and overlap with the exact wavefunction for the various choices of u_i we have considered here. Our inference is that the optimal and the "left-right" ansatz are qualitatively similar and yield a much smaller SMA gap than the "staggered" ansatz.

The SMA calculations suggest that all the spins are involved in the construction of the first excited state from the ground state. The central spins contribute roughly a third as much in the "optimal solution" and exactly as much as the boundary spins in the "left-right" ansatz. The point to note here is that in either case the contribution of the spins in the interior is not small. This suggests that the antiferromagnetic bonds between successive shells do a reasonable job of locking spins together (within each half of the bond centered tree), resulting in an emergent degree of freedom which is what we call a "giant spin". This interpretation will be established next in section VC.

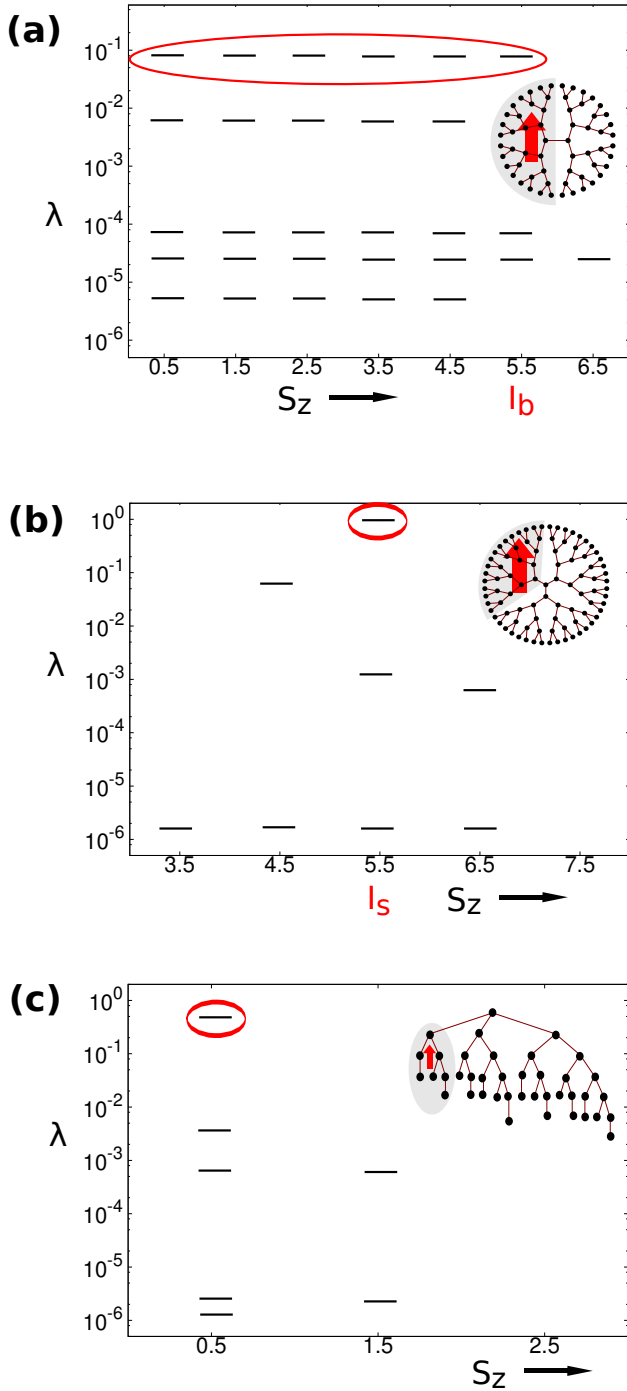


Figure 11: (Color online) The entanglement spectrum for the bond-centered, site-centered and Fibonacci trees as shown in the inset. λ refers to the eigenvalue of the reduced density matrix of the shaded area. The ground state for the bond-centered and Fibonacci clusters was a singlet and only the $S_z > 0$ sectors are shown. For the site-centered cluster we chose to work with the maximal S_z sector (which is the $S_z=16$ for the 94 site cluster). I_b and I_s denote the "imbalance" metric defined in the introduction (refer to Eq.(2.3)). For the bond-centered case, the largest degenerate eigenvalues of the reduced density matrix indicate a multiplet whose spin length exactly equals the imbalance I_b . For the site-centered case, the density matrix has largest weight in a state whose spin is I_s . For the Fibonacci case, a spin 1/2 state has the largest weight in the density matrix.

N_s	u_i	SMA Gap	Overlap
30	Optimal	0.0135	0.998
	Left-Right	0.0341	0.993
	Staggered	0.2680	0.912
62	Optimal	0.0039	0.999
	Left-Right	0.0116	0.997
	Staggered	0.1612	0.946
126	Optimal	0.0010	≈ 1
	Left-Right	0.0028	≈ 1
	Staggered	0.0905	0.975

Table IV: SMA gap and wavefunction overlap with excited state from DMRG for various functional forms of u_i

C. The "Giant Spins" Picture

As we inferred previously, there are indications that strong antiferromagnetic correlations force all spins in one half of the bond-centered cluster to act collectively as a single magnetic moment. We make this understanding more concrete in the present section.

We divide the bond-centered Cayley tree into two equal halves at the central bond. Using the ground state, we compute the reduced density matrix ρ_{RDM} (see Eq.(3.1)) of one of the halves and diagonalize it. The corresponding eigenvalues are arranged by total S_z and the resultant plot is the "entanglement spectrum". The calculation of the entanglement spectrum needs no extra effort in the DMRG procedure we outlined in section III. Appropriate cuts are also chosen for the site-centered and Fibonacci trees as shown in Fig. 11.

The entanglement spectrum shows a copy of the largest eigenvalue in every S_z sector ranging from $-I_b$ to $+I_b$, where I_b is the net sublattice imbalance and is given by $(2^g \pm 1)/6$ as mentioned in equation (2.3). This indicates the presence of a "giant spin" of spin length I_b whose multiplet is given by the eigenvectors corresponding to these large eigenvalues. Given this picture, we explain the existence of the "anomalous" scale of energies.

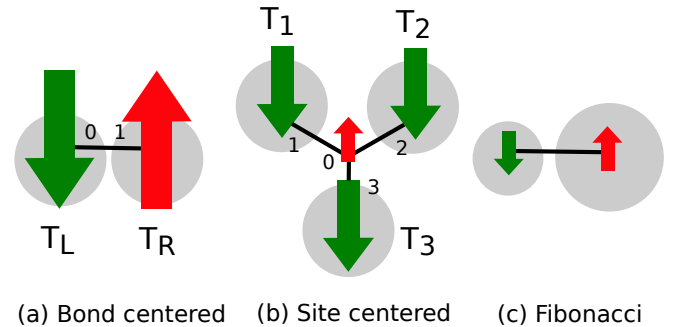


Figure 12: (Color online) The "giant spins" are the low energy degrees of freedom for the bond and site centered clusters that arise out of sublattice imbalance.

1. Bond-centered tree

The Heisenberg Hamiltonian on the bond centered Cayley tree may be rewritten as,

$$H = H_{left} + H_{right} + J\vec{s}_0 \cdot \vec{s}_1 \quad (5.14)$$

We treat the term corresponding to the central bond $J\vec{s}_0 \cdot \vec{s}_1$ as a perturbation within degenerate first order perturbation theory. The many body ground state on each half is a degenerate multiplet of spin I_b . Since all spins on the left and right contribute in a definite proportion to the "giant spin" operators \mathbf{T}_L and \mathbf{T}_R , one can re-express the expectation values of the $J\vec{s}_0 \cdot \vec{s}_1$ in terms of \mathbf{T}_L and \mathbf{T}_R . Note that expectation values of the term $J\vec{s}_0 \cdot \vec{s}_1$ are computed in the product basis of the two systems given by $|T_L, T_L^z\rangle \otimes |T_R, T_R^z\rangle$

If all the spins in one half of the cluster had equal participation in their collective multiplet (observed in the entanglement spectrum), then,

$$\langle T_L, T_L^z | \vec{s}_o | T_L, T_L'^z \rangle = - \langle T_L, T_L^z | \vec{s}_e | T_L, T_L'^z \rangle \quad (5.15)$$

where e (o) refers to *any* even(odd) sublattice site in the same half of the bond centered cluster. Therefore, if one were to create the equally weighted spin operator $\mathbf{T}_L = \sum_i \vec{s}_i$ and consider its matrix elements one would get,

$$\langle \mathbf{T}_L \rangle = \pm 2I_b \langle \vec{s}_0 \rangle \quad (5.16)$$

where 0 refers to the central site in one half of the bond centered cluster. The sign depends on whether the central site and the boundary sites are on the same (+) or opposite (−) sublattices.

What happens when the spins are not equally participating in the multiplet? The simplifying assumption we make here is that within the projected low energy subspace, each individual spin half operator at lattice site i , \vec{s}_i , is proportional to the operator \mathbf{T}_L/I_b . Using the fact that $I_b \sim N_s$, this relation can be expressed as,

$$\vec{s}_0 = \frac{\gamma_b}{N_s} \mathbf{T}_L \quad (5.17)$$

where the constant γ_b has been used to denote the proportionality factor. A similar relation exists for \vec{s}_1 and \mathbf{T}_R . From equation (5.17) it follows that,

$$J \langle \vec{s}_0 \cdot \vec{s}_1 \rangle = \frac{J\gamma_b^2}{N_s^2} \langle \mathbf{T}_L \cdot \mathbf{T}_R \rangle \quad (5.18)$$

The Hamiltonian $\mathbf{T}_L \cdot \mathbf{T}_R$ is diagonalized by coupling the left and right "giant spins" into a spin for the whole system i.e. $\mathbf{T} = \mathbf{T}_L + \mathbf{T}_R$, whose eigenstates are given by $|T, T^z\rangle$.

$$\langle \mathbf{T}_L \cdot \mathbf{T}_R \rangle_{|T, T^z\rangle} = \frac{1}{2} \langle \mathbf{T}^2 - \mathbf{T}_L^2 - \mathbf{T}_R^2 \rangle \quad (5.19)$$

$$= \frac{1}{2} T(T+1) - I_b(I_b+1) \quad (5.20)$$

where T varies from 0, 1, ..., $2I_b$. Note that T_L and T_R are constant and equal to I_b . The term $I_b(I_b+1)$ is a harmless

constant energy shift to all states. Thus, the energy spectrum (up to a overall shift) as a function of T is simply,

$$E(T) = \frac{J\gamma_b^2}{2N_s^2} T(T+1) \quad (5.21)$$

This is exactly the Hamiltonian of a quantum rotor with a "anomalous" moment of inertia scaling as N_s^2 . This simple picture, hence, rather remarkably explains our numerical observations in section IV of the paper. We find γ_b to be ~ 3.24 from fits to our numerical data based on Fig. 7.

Note that though the giant spins are interacting via a weak bond, the fact that they are paired up in a singlet ground state makes the state highly entangled. In comparison, as we shall soon see, the ground state of the site-centered tree (in the $S_z = S_0$ sector) is closer to a product state of the giant spins and hence has a lower degree of entanglement. (This also explains why the convergence of DMRG calculations is more rapid with the number of states M for the site-centered case as compared to the bond-centered case.)

2. Site-centered tree

Let us now perform essentially the same analysis for the site centered Cayley tree to further shed light on (and validate!) the "giant spins" picture. Rewriting the Heisenberg Hamiltonian as,

$$H = H_1 + H_2 + H_3 + J\vec{s}_0 \cdot (\vec{s}_1 + \vec{s}_2 + \vec{s}_3) \quad (5.22)$$

As before, make the substitution of $\vec{s}_1, \vec{s}_2, \vec{s}_3$ in terms of the giant spins $\mathbf{T}_1, \mathbf{T}_2, \mathbf{T}_3$ each of which has spin length I_s . Then couple the three giant spins into a bigger giant spin \mathbf{T} . The Hamiltonian now reads as,

$$H = H_1 + H_2 + H_3 + \frac{J\gamma_s}{N_s} \vec{s}_0 \cdot \mathbf{T} \quad (5.23)$$

where γ_s is a constant and $\mathbf{T} = \mathbf{T}_1 + \mathbf{T}_2 + \mathbf{T}_3$. Note that the angular momentum coupling rules predict that the value of T are in the range from 0, 1... to $3I_s$.

Let us now couple the giant spin \mathbf{T} to the spin 1/2 degree of freedom at the center of the cluster. The energy (in units of $J\gamma_s/N_s$ and up to a constant of $-\frac{3}{4}$) for the $S = 3I_s + \frac{1}{2}$ and $3I_s - \frac{1}{2}$ states is given by,

$$E_{3I_s+\frac{1}{2}}^{3I_s+\frac{1}{2}} = \left(3I_s + \frac{1}{2}\right) \left(3I_s + \frac{3}{2}\right) - 3I_s(3I_s+1) \quad (5.24a)$$

$$E_{3I_s-\frac{1}{2}}^{3I_s-\frac{1}{2}} = \left(3I_s - \frac{1}{2}\right) \left(3I_s + \frac{1}{2}\right) - 3I_s(3I_s+1) \quad (5.24b)$$

where the superscript indicates the global value of the spin S and the subscript is used to indicate the T value it was made

of. Similarly we have,

$$E_{3I_s-1}^{3I_s-\frac{1}{2}} = \left(3I_s - \frac{1}{2}\right) \left(3I_s + \frac{1}{2}\right) - 3I_s(3I_s - 1) \quad (5.25a)$$

$$E_{3I_s-1}^{3I_s-\frac{3}{2}} = \left(3I_s - \frac{3}{2}\right) \left(3I_s - \frac{1}{2}\right) - 3I_s(3I_s - 1) \quad (5.25b)$$

Simplifying equations and incorporating the constant of $-\frac{3}{4}$ we get,

$$E_{3I_s}^{3I_s+\frac{1}{2}} = 3I_s \quad (5.26a)$$

$$E_{3I_s}^{3I_s-\frac{1}{2}} = -3I_s - 1 \quad (5.26b)$$

$$E_{3I_s-1}^{3I_s-\frac{1}{2}} = 3I_s - 1 \quad (5.26c)$$

$$E_{3I_s-1}^{3I_s-\frac{3}{2}} = -3I_s \quad (5.26d)$$

Observe that $E_{3I_s}^{3I_s-\frac{1}{2}}$ is the lowest energy. This is in concordance with the Lieb-Mattis theorem³⁴ i.e. the ground state has total spin $S_0 = 3I_s - \frac{1}{2}$. The energy gap (now in absolute units) of the S_0 to $S_0 + 1$ transition is given by,

$$\Delta(S_0 \rightarrow S_0 + 1) = \frac{J\gamma_s}{N_s} (6I_s + 1) \quad (5.27)$$

Since I_s is approximately $N_s/18$ for large N_s we get a gap of,

$$\Delta(S_0 \rightarrow S_0 + 1) \approx \frac{J\gamma_s}{3} \quad (5.28)$$

This is consistent with our numerical observation that the gap is finite in the large N_s limit. Since the measured gap is $\sim 0.73J$ we infer that γ must be ~ 2.19 .

We give further credibility to our giant spin interpretation by testing the prediction of the gap for the S_0 to $S_0 - 1$ transition. This turns out to be gapless in the large N_s limit,

$$\Delta(S_0 \rightarrow S_0 - 1) \approx \frac{J\gamma_s}{N_s} \quad (5.29)$$

which is consistent with our DMRG calculations as shown in Fig. 13. The measured γ_s from the fit of the DMRG data to $\Delta = J\gamma_s/N_s$ is found to be ~ 2.19 consistent with the estimate from equation (5.28), serving as another check of the theory.

3. Fibonacci Cayley tree

The entanglement spectrum of the Fibonacci Cayley tree (see Fig. 11(c)) indicates the creation of a spin 1/2 degree of freedom as opposed to the "giant spins" encountered previously. The cut shown in Fig. 11(c) shows a region having an imbalance of one, which is the maximum possible for any cut.

We believe the lowest energy excitation of this system involves a breaking of a dimer and creation of two unpaired

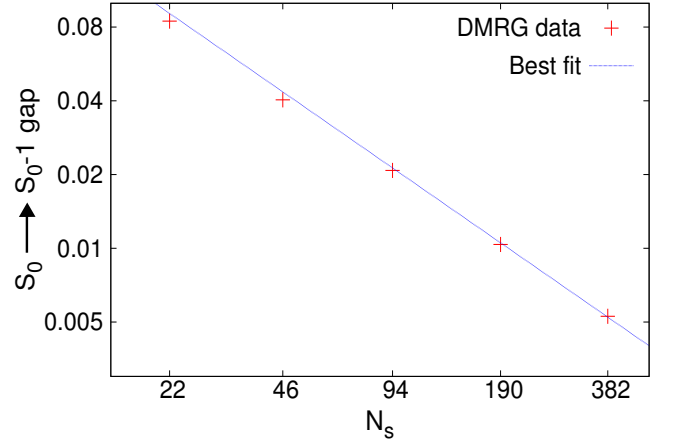


Figure 13: (Color online) For the site centered clusters, the scaling of the S_0 to $S_0 - 1$ energy gap serves as one of the test beds for the "giant spins" picture presented in the text. Here we see a reasonable agreement of the DMRG data with the predicted scaling of $1/N_s$.

spins. Since the bonds in the interior have a decreasing dimerization strength, the energy required to create this excitation is expected to be vanishingly small in the infinite lattice limit. This is seen in the spin gap in Table III, but an explanation of the observed numerical exponent is a subject of further investigation.

VI. SCHWINGER BOSON MEAN FIELD THEORY FOR SINGLET GROUND STATES

Can we understand the presence or absence of long range order on these trees at the mean field level? For this we appeal to the Schwinger Boson Mean Field Theory⁵ which is capable of describing quantum disordered and ordered states within the same framework^{4,40}. In this section we will see that this theory is a good description of the singlet ground states of the bond centered and Fibonacci trees. This section also serves to expand the domain of application of the Schwinger Boson formalism to situations where multiple parameters need to be optimized simultaneously⁴¹ (such as non uniform systems or systems with very few symmetries).

A. Notation and formal set-up

The $SU(N)$ Heisenberg Hamiltonian is expressed in terms of Schwinger Bosons by defining a bond operator,

$$\mathcal{A}_{ij} = \sum_{m=1}^N b_{im} b_{jm} \quad (6.1)$$

where each Schwinger boson operator b_{im} carries two labels, i or j for site indices and m for flavor index. The physical Heisenberg model Eq.(2.1) corresponds to $N = 2$. The procedure is to decouple the quartic bosonic Hamiltonian into a one-body mean field Hamiltonian by doing an expansion

in $1/N$. Solving the mean field Hamiltonian and putting in $N = 2$ allows us to compare the SBMFT results with DMRG calculations.

The $SU(N)$ Hamiltonian in terms of Schwinger bosons is,

$$\mathcal{H}_{Heis.} = -\frac{J}{N} \sum_{\langle ij \rangle} (\mathcal{A}_{ij}^\dagger \mathcal{A}_{ij} - 2S^2) \quad (6.2)$$

The mapping of the spin Hamiltonian to Schwinger bosons is exact if we meet the condition site by site,

$$\sum_{m=1}^N b_{im}^\dagger b_{im} = NS \quad (6.3)$$

which ensures that the Hilbert space of the bosons is restricted by the spin size S (and the corresponding $|S, S_z\rangle$ states). However, we will impose this constraint only on the expectation $b_{im}^\dagger b_{im} \rightarrow \langle b_{im}^\dagger b_{im} \rangle_{MF}$. As a result of not satisfying Eq.(6.3) exactly, the mean field energy E_{MF} and correlations differ from exact results (DMRG calculations) by overall scale factors^{5,42}.

The decoupled mean field Hamiltonian \mathcal{H}_{MF} is expressed in terms of the following variational parameters: a set of bond variables Q_{ij} for every bond i, j , Lagrange multipliers λ_i which impose Eq.(6.3) and a condensate field $\beta_i = \delta_{1,m} \langle b_{im} \rangle / \sqrt{N}$ which develops a non-zero value in a phase with LRO⁴⁰. \mathcal{H}_{MF} is then given by,⁶

$$\begin{aligned} \mathcal{H}_{MF} = & \sum_{i=1}^{N_s} \lambda_i \left(\sum_{m=1}^N b_{im}^\dagger b_{im} - NS \right) + \frac{N}{J} \sum_{\langle ij \rangle} |Q_{ij}|^2 \\ & + \sum_{i < j} \left(Q_{ij} \mathcal{A}_{ij}^\dagger + Q_{ij}^* \mathcal{A}_{ij} \right) \\ & + \frac{1}{\sqrt{N}} \sum_{i=1}^{N_s} \left(\phi_i^* b_{i1} + \phi_i b_{i1}^\dagger \right) \end{aligned} \quad (6.4)$$

The field ϕ_i couples linearly to Schwinger bosons and is conjugate to $\delta_{1,m} \langle b_{im}^\dagger \rangle$. As a result of this parametrization, the lowest spinon frequency mode ω_0 of the $m = 1$ flavor develops a macroscopic occupation of Schwinger bosons on Bose condensation. At the mean field level the different boson flavors decouple and the part of the mean field Hamiltonian quadratic in bosonic operators b_{im}, b_{im}^\dagger ($m = 2, \dots, N$) can be expressed as $N - 1$ copies of a quadratic Hamiltonian \mathcal{H}_{MF}^m . \mathcal{H}_{MF}^m is given by,

$$\mathcal{H}_{MF}^m = \sum_{i=1}^{N_s} \lambda_i b_{im}^\dagger b_{im} + \sum_{i < j} \left(Q_{ij} b_{im}^\dagger b_{jm}^\dagger + \text{h.c.} \right) \quad (6.5)$$

Integrating out the bosonic fields then gives us a set of single-spinon frequency modes and the total mean field energy E_{MF} . Since we do not have the luxury of momentum space, we adopt a real space Bogoliubov diagonalization procedure⁴³. Since \mathcal{H}_{MF}^m is block diagonal in the flavor basis

(the Hamiltonian is the same for all $N - 1$ flavors) we can now drop the flavor index m and express it as

$$\mathcal{H}_{MF}^m = \frac{1}{2} \begin{pmatrix} \mathbf{b}^\dagger & \mathbf{b} \end{pmatrix} \begin{pmatrix} \Lambda & Q \\ Q & \Lambda \end{pmatrix} \begin{pmatrix} \mathbf{b} \\ \mathbf{b}^\dagger \end{pmatrix} \quad (6.6)$$

where $m \neq 1$, $\mathbf{b} = (b_1, b_2, \dots, b_{N_s})$ and Λ and Q are $N_s \times N_s$ matrices given by $\Lambda_{ij} = \lambda_i \delta_{ij}$ and $Q_{ij} = Q_{ij}$ for nearest neighbor sites i, j . \mathcal{H}_{MF}^m can now be diagonalized by introducing Bogoliubov transformation matrices, \mathbf{U} and \mathbf{V} defined as follows,

$$\begin{pmatrix} \mathbf{b} \\ \mathbf{b}^\dagger \end{pmatrix} = \begin{pmatrix} \mathbf{U} & \mathbf{V} \\ \mathbf{V}^* & \mathbf{U}^* \end{pmatrix} \begin{pmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\alpha}^\dagger \end{pmatrix} \quad (6.7)$$

where $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \dots, \alpha_{N_s})$ is a vector of Bogoliubov quasiparticle annihilation operators. Each quasiparticle creation (annihilation) operator α_μ^\dagger (α_μ) creates (destroys) a bosonic quasiparticle in the single particle mode μ , where μ goes from 1 to N_s . The transformation (6.7) allows us to switch to the Bogoliubov quasiparticle basis where \mathcal{H}_{MF}^m becomes,

$$\mathcal{H}_{MF}^m = \sum_{\mu=1}^{N_s} \omega_\mu \left(\alpha_\mu^\dagger \alpha_\mu + \frac{1}{2} \right) \quad (6.8)$$

We can now do a Legendre transformation to replace the field ϕ_i by β_i , allowing us to express E_{MF} as,

$$\frac{E_{MF}}{N} = \sum_{\mu=1}^{N_s} \frac{1}{2} \omega_\mu + \frac{1}{J} \sum_{i < j} |Q_{ij}|^2 - \left(S + \frac{1}{2} \right) \sum_{i=1}^{N_s} \lambda_i + E_{cond} \quad (6.9)$$

and E_{cond} is given by,

$$E_{cond} = \sum_{i=1}^{N_s} \lambda_i |\beta_i|^2 + \sum_{i < j} (Q_{ij} \beta_i^* \beta_j^* + \text{h.c.}) \quad (6.10)$$

We now consider the case of $N = 2$. The variational parameters $\{\lambda_i\}$, $\{Q_{ij}\}$ and $\{\beta_i\}$ are determined by minimizing E_{MF} with respect to each of them giving the following constraints,

$$\frac{\partial E_{MF}}{\partial \lambda_i} = 0 \Rightarrow |\beta_i|^2 + \langle b_{i2}^\dagger b_{i2} \rangle = S \quad (6.11a)$$

$$\frac{\partial E_{MF}}{\partial Q_{ij}} = 0 \Rightarrow \beta_i^* \beta_j^* + \frac{\langle \mathcal{A}_{ij} \rangle}{N} + \frac{1}{J} Q_{ij} = 0 \quad (6.11b)$$

$$\frac{\partial E_{MF}}{\partial \beta_i} = 0 \Rightarrow \lambda_i \beta_i^* + \sum_{j \text{ n.n. } i} Q_{ij}^* \beta_j^* = 0 \quad (6.11c)$$

One of the obvious considerations of applying this theory to such a non-uniform lattice is the large number of variational parameters which, in general, scale with the system size N_s . However, due to the symmetries of the Cayley tree the number of independent parameters are reduced to order g . The task then is to find an optimal set of parameters $\{\lambda_i^*, Q_{ij}^*, \beta_i^*\}$ which satisfy the constraints in (6.11a), (6.11b) and (6.11c). This is done numerically and is discussed in subsection C.

The resulting optimal $E_{MF}(\lambda_i^*, Q_{ij}^*, \beta_i^*)$ can be related to the physical Heisenberg energy via,

$$E_{Heis.} = 2E_{MF} + \sum_{\langle ij \rangle} JS^2 \quad (6.12)$$

A note on the β_i minimization constraint (6.11c): a trivial solution of this equation is to choose $\beta_i = 0$ for all sites. This is the quantum disordered phase. A non zero value of β_i signals condensation of Schwinger bosons and long range order.

For finite uniform systems there is no spontaneous symmetry breaking and correspondingly no condensation of bosons⁴⁴. Introduction of the condensate field β_i is analogous to applying a staggered field in the system that couples to the staggered magnetization. This breaks the degeneracy of the single particle energies corresponding to the two boson flavors (for $N = 2$). The condensate fraction begins to build up in the flavor mode with the lowest frequency.

The algorithm tries to initially find a self-consistent mean field solution by varying only the set of λ_i and Q_{ij} 's. However, if we cannot satisfy the constraints in equations (6.11a, 6.11b) (with $\beta_i = 0$), we resort to adding the condensate field β_i , as an additional set of variational parameters. While we can not completely rule out the possibility of a solution with $\beta_i = 0$, we believe that the appearance of a condensate is *physical*.

B. Correlation functions in Quantum disordered and LRO phase

Here we compute correlation functions that enter into the self consistency equations (6.11a, 6.11b, 6.11c). The boson density of a given flavor at site i is given by (suppressing the flavor index),

$$\begin{aligned} \langle b_i^\dagger b_i \rangle &= \sum_{p,q=1}^{N_s} \langle (\mathbf{U}_{ip}^* \boldsymbol{\alpha}_p^\dagger + \mathbf{V}_{ip}^* \boldsymbol{\alpha}_p) (\mathbf{U}_{iq} \boldsymbol{\alpha}_q + \mathbf{V}_{iq} \boldsymbol{\alpha}_q^\dagger) \rangle \\ &= \sum_{p,q=1}^{N_s} \mathbf{V}_{ip}^* \mathbf{V}_{iq} \langle \boldsymbol{\alpha}_p \boldsymbol{\alpha}_q^\dagger \rangle \\ &= (\mathbf{V}^* \mathbf{V}^T)_{ii} \end{aligned} \quad (6.13)$$

The indices p, q run over all single particle modes and we made use of $\langle \boldsymbol{\alpha}_p \boldsymbol{\alpha}_q^\dagger \rangle = \delta_{p,q}$ which follows since the SBMFT many body ground state is the vacuum of Bogoliubov quasiparticles. Similarly,

$$\langle b_i b_j \rangle = (\mathbf{U} \mathbf{V}^T)_{ij} \quad (6.14)$$

Spin correlation functions G_{ij} can be computed in a similar fashion. The only complication arises in the $SU(2)$ broken symmetry phase where, due to loss of spin rotational invariance, we need to compute the $\langle S_i^z S_j^z \rangle$ correlations. This involves evaluating a quartic expectation which we decouple into a series of 2 point functions using Wick's theorem. For

simplicity of notation we define the following combinations of \mathbf{U} and \mathbf{V} matrices,

$$\begin{aligned} \tilde{\mathbf{Q}} &\equiv \mathbf{U} \mathbf{V}^T \\ \tilde{\mathbf{U}} &\equiv \mathbf{U} \mathbf{U}^\dagger \\ \tilde{\mathbf{V}} &\equiv \mathbf{V} \mathbf{V}^T \end{aligned} \quad (6.15)$$

Spin correlations in the Quantum disordered and the broken symmetry LRO phase are then given by,

$$\begin{aligned} (G_{ij})_{Q.dis.} &= \begin{cases} -\frac{3}{2} \tilde{\mathbf{Q}}_{ij}^\dagger \tilde{\mathbf{Q}}_{ij} & \text{for } i \in A, j \in B \\ \frac{3}{2} \tilde{\mathbf{V}}_{ij} \tilde{\mathbf{U}}_{ij} & \text{for } (i, j) \in A \text{ or } B \end{cases} \quad (6.16a) \\ (G_{ij})_{LRO} &= \begin{cases} -N \beta_i \beta_j \tilde{\mathbf{Q}}_{ij} - \frac{1}{4} \tilde{\mathbf{Q}}_{ij}^\dagger \tilde{\mathbf{Q}}_{ij} & \text{for } i \in A, j \in B \\ \frac{1}{2} N \beta_i \beta_j (\tilde{\mathbf{U}} + \tilde{\mathbf{V}})_{ij} + \frac{1}{4} \tilde{\mathbf{V}}_{ij} \tilde{\mathbf{U}}_{ij} & \text{for } (i, j) \in A \text{ or } B \end{cases} \quad (6.16b) \end{aligned}$$

In the quantum disordered phase SBMFT overestimates G_{ij} by an overall scale factor⁵ of 3/2. We normalize the SBMFT correlation function by this factor to take into account the $1/N$ fluctuation effects for $N = 2$. Similarly, in the phase with LRO we find that we need to scale up G_{ij} by a factor of 1.8 to make it agree quantitatively with DMRG results. Similar overall scale factors have been reported previously⁴². These overall scale factors can be suppressed by using Gutzwiller projected mean field wavefunctions⁴⁵, which is feasible only for small system sizes. Such projected wavefunctions have also been shown to give energies in agreement with exact results^{42,45}.

C. Numerical Implementation

Using the symmetry of the bond-centered Cayley tree, we reduce the number of variational mean field parameters. A first simplification results from the fact that all sites within a given shell on the lattice are equivalent and are therefore assigned the same λ_i and β_i . Similarly, all bonds connecting two successive shells are equivalent and have the same Q'_{ij} 's. For the Fibonacci cluster there are fewer exact symmetries (only reflection about the central bond) compared to the Cayley tree and therefore a larger number of variational parameters are required.

We use the Nelder Mead Simplex optimizer from the GSL library to minimize the following weighted combined cost function which aims to reduce (6.9) subject to the constraints (6.11a), (6.11b) and (6.11c). Since each of these constraint equations are obtained by minimizing (6.9) with respect to the variational parameters λ_i , Q_{ij} and β_i , enforcing the constraints will minimize E_{MF} .

$$C(\{\lambda_i\}, \{Q_{ij}\}, \{\beta_i\}) = \mu_0 C_\lambda + \mu_1 C_Q + \mu_2 C_\beta \quad (6.17)$$

where $\{\mu_0, \mu_1, \mu_2\}$ are relative weights of terms in the cost function and the costs are given by,

$$C_\lambda = \sum_{i=1}^{N_s} \left((|\beta_i|^2 + \langle b_{i2}^\dagger b_{i2} \rangle) - S \right)^2 \quad (6.18a)$$

$$C_Q = \sum_{i < j} \left(\beta_i \beta_j + \frac{1}{N} \langle \mathcal{A}_{ij} \rangle + \frac{1}{J} Q_{ij} \right)^2 \quad (6.18b)$$

$$C_\beta = \sum_{i=1}^{N_s} \left(\lambda_i \beta_i^* + \sum_{j \text{ n.n. } i} Q_{ij}^* \beta_j^* \right)^2 \quad (6.18c)$$

In practice, to minimize the weighted cost function (6.17), tolerance values for the C_β and C_λ are set at 10^{-8} and 10^{-14} respectively and the Q_{ij} 's are solved for self-consistently. A good initial guess for the Q_{ij} 's is a pattern that favors dimerization as suggested by results from Exact Diagonalization for small clusters. A good rule of thumb for the bond centered cluster is to begin by dimerizing (assigning a high value of Q_{ij}) the outermost bond and to create a pattern, moving inwards, of alternating bond strengths.

For cases requiring a larger number of variational parameters (like in the case of the Fibonacci cluster) it helps to guide the Nelder Mead optimization using a "relaxation" algorithm. The algorithm starts with an initial guess for the Q_{ij} 's and allows the optimizer to find an optimal set of λ_i 's. If the tolerance level for C_λ is not met, the Q_{ij} 's are allowed to relax: i.e. the best set of λ_i 's is taken as initial guess in an optimization where the Q_{ij} 's are now taken to be the variational parameters. Thus, by alternating in the choice of variational parameters between λ_i 's and the Q_{ij} 's for each optimization cycle we converge to the desired tolerance limit.

The stability of the obtained mean field solution was checked by adding small random perturbations to the optimal mean field parameters. In the quantum disordered phase, the saddle point was checked to correspond to a maximum in λ_i 's and a minimum in the Q_{ij} 's.

Every optimization cycle scales as $\sim N_s^3 \tau$, where τ is the total time for functional evaluation taken by the optimizer to converge to a solution. A typical optimization time for the $N_s=126$ cluster is about 20 minutes on a personal workstation (2.7 GHz Intel Core i7).

D. Results

The landscape of the cost function (6.17) in parameter space has many local minima with very similar mean field energies (differing by 1% or less). As a result, we get a zoo of physically plausible mean field solutions, all of which satisfy (6.11a) and have comparable E_{MF} . To choose the optimal solution from amongst those, we look at the β_i minimization constraint (6.11c) and hand pick the one which has the lowest C_β . In other words, the chosen solution has the lowest spinon frequency ω_0 .

The mean field energy and correlation functions for the bond-centered Cayley trees suffer from significant finite size

effects (number of sites on the boundary scales as the system size N_s). As a result, for the finite systems considered above, the lowest spinon frequency is always gapped $\omega_0 \neq 0$ in spite of a very low $\beta_{cost} (\sim 10^{-8})$. However, with increasing system size, ω_0 lowers and spinons begin to condense in this lowest frequency mode. Fig. 14 shows a finite size fit to the lowest spinon mode. Spinon condensation and a very small ω_0 suggest long range order in the thermodynamic limit.

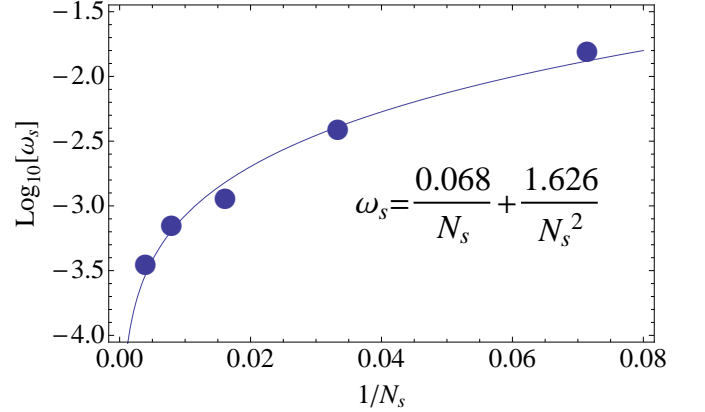


Figure 14: (Color online) The lowest spinon frequency appears to go to 0 as $1/N_s$. This signals appearance of long range order within the Schwinger Boson Theory.

Since condensation of spinons signals long range order, sites with a higher condensate fraction have a greater participation in establishing Neel order on the cluster. By mapping out the condensate fraction on different radial shells in Fig. 15(b) we notice the strong correspondence between sites with large condensate densities and those with a high "flippability" as in Eq.(5.8).

Our results can be put in perspective with respect to a heuristic for computing the number of "dangling spins" proposed by Wang and Sandvik¹³ in the context of percolation clusters on the square lattice. We "dimerize" the lattice maximally as shown in Fig. 15(a) and the spins that remain are called "dangling". These are the representative spins participating as the low energy degrees of freedom. (Note that the choice of maximal dimer covering is not unique but the number of uncovered spins is the same in all such coverings)

VII. CONCLUSION

In this paper, we have explored the relationship between sublattice imbalance and nature of the low energy spectrum of the bond-centered, site-centered and Fibonacci Cayley trees.

For the bond-centered Cayley tree, we find that the spin gap scales with size as $1/N_s^\alpha$ where α was found to be ≈ 2 . We discover an entire tower of states (Fig. 6) with a much larger moment of inertia (Fig. 7) than the Anderson Tower of States. This low energy scale persists up to a spin value of $S^* = 2I_b$, where I_b refers to a measure of the imbalance (or the number of "unpaired spins") on the bond centered tree (as in Eq.(2.3)).

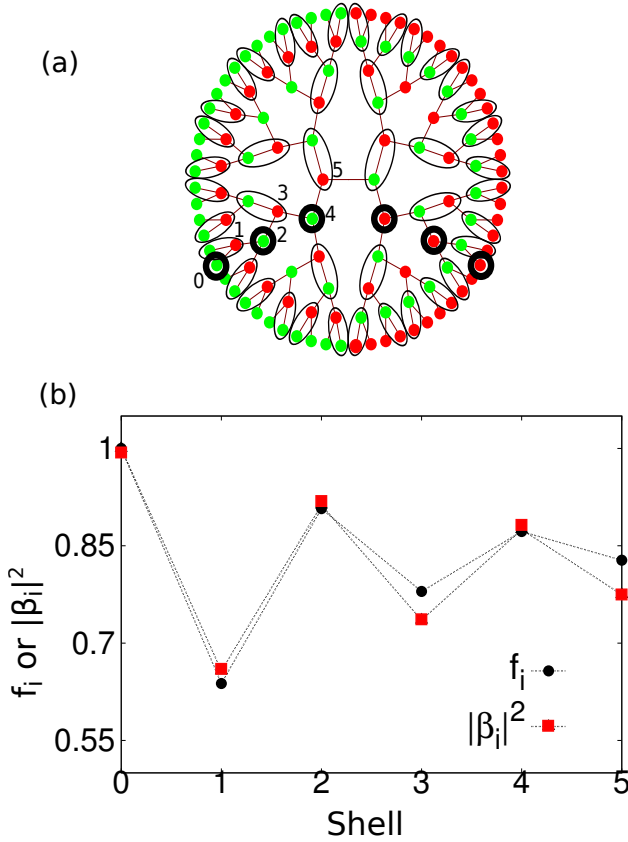


Figure 15: (Color online) Above (a): Heuristic for computing the number of "dangling spins" as proposed by Wang and Sandvik. Below (b): The "flippability" as in Eq.(5.8) computed from DMRG and the condensate fraction $|\beta_i|^2$ computed from SBMFT on every shell of the bond centered Cayley tree. Both quantities are qualitatively consistent with each other and confirm the "dangling" spin heuristic shown above.

To highlight the role of sublattice imbalance, we introduced the Fibonacci Cayley tree in sec. II, which does not have any locally unpaired spins. We found it lacks the low lying states characteristic of the bond-centered tree (see Fig. 6). Instead, the spin gap vanishes as $\approx 1/N_s^{0.6}$. However, both trees have similar susceptibilities ($\sim N_s$) at sufficiently large magnetic fields. This is because the strength of the dimerization is relatively weak at sufficiently high energy scales (comparable to J), allowing all spins to lock together, leading to an extensive susceptibility.

For the site centered tree, our results are in good agreement with a recent study²². We report a finite spin gap of $\Delta = 0.731(4)$ in the infinite lattice limit and a ground state energy of $e_0 = -0.393854(1)$.

Our results can be explained within a unifying framework of individual spins coupling together to form collective spin degrees of freedom which we refer to as "giant spins". The idea for coupling big sublattice spins is well known¹⁵ in the context of regular lattices. However, we emphasize that the "giant spins" are created by coupling all spins (both even and odd sublattice spins) in regions with large local sublattice imbalances. For the bond- and site-centered lattices, we find

that all lattice sites have a (nearly) uniform participation in the "giant spins". This picture is verified by two independent techniques in section V - the single mode approximation for the excited state and an observation of the entanglement spectrum.

In a broader context, our study aims to understand the nature of unpaired spins coupling in a strongly dimerized background. Such spins, termed as "dangling spins", have been predicted from numerical simulations¹³ for systems with quenched random dilution. Thus, a natural extension of our study is to consider such dangling spins on percolation clusters where we expect that they couple hierarchically to form emergent giant spins at different length scales. This will be the subject of a future publication³⁶.

In this paper, we have explored several techniques to develop our understanding. To begin with, we obtain accurate many-body wavefunctions and their expectations using an implementation of the Density Matrix Renormalization Group (DMRG) procedure (described in section III) that works for generic trees. In general, this procedure is expected to be well suited to hierarchical lattices and those with few or no loops, such as the Husimi Cactus^{46,47}, a lattice of corner sharing triangles (dual to the Cayley tree and locally like the Kagome Lattice).

To have an understanding at the mean field level, we adapted Schwinger Boson Mean Field Theory (SBMFT) to a larger number of variational parameters than considered previously^{42,45,48}. We were able to study spin correlations of the bond-centered and Fibonacci trees (singlet ground states). Rather remarkably, the theory is quite accurate *quantitatively* in predicting ground state spin-spin correlation functions (see Fig. 5), up to overall multiplicative scale factors (as discussed in section VI). The recipe outlined in section VI can be used to navigate through the zoo of feasible mean field solutions by giving relative weights to the constraint equations (6.18a, 6.18b, 6.18c).

We believe that most applications of SBMFT have focused on quantum disordered phases^{49,50}, but the broken symmetry phase has received less attention. The setup can also be generalized to handle frustrated spin systems without the need to have an ansatz for the mean field fluxes or the decoupling parameters⁴⁹. This might lead to novel spin liquid ground states with new kinds of broken symmetries⁴¹.

After writing this paper, we came across recent results by G.Misguich⁴¹, who has done an extensive numerical study of SBMFT formalism for spatially inhomogenous states, mostly concentrating on gapped systems. However, his study differs from ours in that we include the condensate field as a variational parameter. It will be interesting to apply our formalism to further investigate his proposed set of ground states.

VIII. ACKNOWLEDGMENT

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Appendix A: Derivation of the SMA gap equation for the Heisenberg Model

In section V, we introduced the single mode approximation (SMA) for the excited state in terms of the ground state,

$$|1'\rangle = \sum_i u_i s_i^+ |0\rangle \quad (\text{A.1})$$

where $|0\rangle$ is the singlet ground state and $|1'\rangle$ is the approximate triplet excited state. i refers to a site index. In this Appendix, we will derive an expression for the SMA energy gap Δ_{SMA} in terms of the ground state correlations and the parameters u_i .

The expression for the gap between the ground and first excited state is,

$$\Delta = \frac{\langle 1' | H | 1' \rangle}{\langle 1' | 1' \rangle} - E_0 \quad (\text{A.2})$$

where E_0 is the ground state energy. Plugging in the expression for $|1'\rangle$ from equation (A.1) we have,

$$\Delta_{SMA} = \frac{\langle 0 | \sum_{ij} u_i u_j s_j^- H s_i^+ | 0 \rangle}{\langle 0 | \sum_{ij} u_i u_j s_j^- s_i^+ | 0 \rangle} - E_0 \quad (\text{A.3})$$

$$= \frac{\sum_{ij} u_i u_j \langle s_j^- [H, s_i^+] \rangle}{\sum_{ij} u_i u_j \langle s_j^- s_i^+ \rangle} + \frac{\sum_{ij} u_i u_j \langle s_j^- s_i^+ H \rangle}{\sum_{ij} u_i u_j \langle s_j^- s_i^+ \rangle} - E_0 \quad (\text{A.4})$$

$$= \frac{\sum_{ij} u_i u_j \langle s_j^- [H, s_i^+] \rangle}{2 \sum_{ij} u_i u_j \langle s_j^z s_i^z \rangle} \quad (\text{A.5})$$

Next, consider the nearest neighbor Heisenberg Hamiltonian,

$$H = \frac{J}{2} \sum_{\langle k, l \rangle} \left(s_k^z s_l^z + \frac{1}{2} (s_k^+ s_l^- + s_k^- s_l^+) \right) \quad (\text{A.6})$$

where $\langle k, l \rangle$ refer to nearest neighbor pairs. We have included a factor of 1/2 outside to compensate for counting each nearest neighbor term twice.

We now calculate $[H, s_i^+]$ occurring in Eq.(A.5). To do so, we calculate $[\vec{s}_k \cdot \vec{s}_l, s_i^+]$ as,

$$\begin{aligned} [\vec{s}_k \cdot \vec{s}_l, s_i^+] &= s_k^z [s_l^z, s_i^+] + s_l^z [s_k^z, s_i^+] + \\ &\quad \frac{1}{2} s_k^+ [s_l^-, s_i^+] + \frac{1}{2} [s_k^-, s_i^+] s_l^+ \\ &= \delta_{il} s_k^z s_l^+ + \delta_{ik} s_l^z s_k^+ \\ &\quad - \delta_{il} s_k^+ s_l^z - \delta_{ik} s_k^z s_l^+ \end{aligned} \quad (\text{A.7})$$

The numerator of Eq.(A.5) involves the term $\langle s_j^- [H, s_i^+] \rangle$. Hence we now consider the action of the s_j^- operator on the simplified expression for $[\vec{s}_k \cdot \vec{s}_l, s_i^+]$ in Eq.(A.7). Consider only the terms that have $j = k$ or $j = l$ (since $k \neq l$ terms do not occur in the Hamiltonian we do not have to worry about the possibility $j = k = l$). In addition, time reversal symmetry of the ground state wavefunction (equivalent to simply asserting the $S_z \rightarrow -S_z$ symmetry of the ground state) ensures that if both $j \neq k$ and $j \neq l$ then the three point correlation function is exactly 0. This latter point is rather subtle and so we expand on this in Appendix B.

Thus the expression for $s_j^- [\vec{s}_k \cdot \vec{s}_l, s_i^+]$ (after retaining only the $j = k$ and $j = l$ terms) is,

$$\begin{aligned} s_j^- [\vec{s}_k \cdot \vec{s}_l, s_i^+] &= -\delta_{ik} \delta_{jl} \left(\frac{1}{2} - s_l^z \right) s_k^z - \delta_{ik} \delta_{jk} \frac{s_k^- s_l^+}{2} \\ &\quad - \delta_{il} \delta_{jk} \left(\frac{1}{2} - s_k^z \right) s_l^z - \delta_{il} \delta_{jl} \frac{s_l^- s_k^+}{2} \\ &\quad + \delta_{jk} \delta_{il} \frac{s_k^- s_l^+}{2} + \delta_{jl} \delta_{il} \left(\frac{1}{2} - s_l^z \right) s_k^z \\ &\quad + \delta_{jk} \delta_{ik} \left(\frac{1}{2} - s_k^z \right) s_l^z + \frac{1}{2} s_k^+ s_l^- \delta_{ik} \delta_{jl} \end{aligned} \quad (\text{A.8})$$

Inserting (A.8), in the expression for the SMA gap (A.5) for the Heisenberg Hamiltonian and utilizing $\langle s_i^z \rangle = 0$ for all i , we obtain,

$$\Delta_{SMA} = - \frac{\sum_{\langle k, l \rangle} (u_k - u_l)^2 \langle s_k^z s_l^z \rangle}{2 \sum_{ij} u_i u_j \langle s_i^z s_j^z \rangle} \quad (\text{A.9})$$

Appendix B: Why is $\langle \psi | s_j^- s_k^+ s_l^z | \psi \rangle = 0$ for distinct j, k, l ?

To derive the SMA gap equation in Appendix , we used,

$$\langle \psi | s_j^- s_k^+ s_l^z | \psi \rangle = 0 \quad (\text{B.1})$$

for distinct site indices j, k, l . In this Appendix, we will prove this statement for *any* wavefunction which is invariant under time reversal.

Consider three distinct spins i, j, k . Express the wavefunction in the basis spanned by the three spins at sites j, k, l and the rest of the spins (collectively termed as "environment" e),

$$|\psi\rangle = \sum_{s'_j s'_k s'_l} \sum_e w_e^{s'_j s'_k s'_l} |s'_j s'_k s'_l\rangle \otimes |e\rangle \quad (\text{B.2})$$

Since this wavefunction is an eigenstate of the Heisenberg model (with no external magnetic fields), it follows that under time reversal (denoted by operator T) we have,

$$\psi \rightarrow z\psi \quad (\text{B.3})$$

where z is ± 1 .

This implies that the coefficients in the wavefunction satisfy the relation,

$$w_e^{s'_j s'_k s'_l} = z w_{-e}^{-s'_j -s'_k -s'_l} \quad (\text{B.4})$$

The action of the operator $s_j^- s_k^+ s_l^z$ on $|\psi\rangle$ from Eq.(B.2) yields,

$$s_j^- s_k^+ s_l^z |\psi\rangle = \sum_{s'_l} \sum_e w_e^{\uparrow\downarrow s'_l} |\downarrow\uparrow s'_l\rangle \otimes |e\rangle \quad (\text{B.5})$$

Now acting Eq.(B.5) with $\langle\psi|$ from the left and using the orthogonality of the basis we get,

$$\begin{aligned} \langle\psi| s_j^- s_k^+ s_l^z |\psi\rangle &= \sum_{s'_l} \sum_e w_e^{\uparrow\downarrow s'_l} w_e^{\uparrow\downarrow s'_l} \quad (\text{B.6}) \\ &= \frac{1}{2} \sum_{e_-} w_{e_-}^{\uparrow\uparrow\uparrow} w_{e_-}^{\uparrow\downarrow\uparrow} \\ &\quad - \frac{1}{2} \sum_{e_+} w_{e_+}^{\uparrow\downarrow\downarrow} w_{e_+}^{\uparrow\uparrow\downarrow} \quad (\text{B.7}) \end{aligned}$$

where e_+ (e_-) reflects the fact that the environment carries a net S_z of $+$ ($-$) $\frac{1}{2}$ since the wavefunction comprises of $S_{tot}^z = 0$ terms only. Under inversion of all spins in e_+ we get e_- . With this in mind, consider the second sum on the right. Using the time reversal symmetry of the wavefunction i.e. $w_{e_+}^{\uparrow\downarrow\downarrow} = z w_{e_-}^{\uparrow\uparrow\uparrow}$ and $w_{e_+}^{\uparrow\uparrow\downarrow} = z w_{e_-}^{\uparrow\downarrow\uparrow}$ (as seen from Eq.(B.4)), in Eq.(B.7) we get,

$$\langle\psi| s_j^- s_k^+ s_l^z |\psi\rangle = \frac{1}{2} \sum_{e_-} w_{e_-}^{\uparrow\uparrow\uparrow} w_{e_-}^{\uparrow\downarrow\uparrow} \quad (\text{B.8})$$

$$\begin{aligned} &- \frac{1}{2} z^2 \sum_{e_-} w_{e_-}^{\uparrow\downarrow\uparrow} w_{e_-}^{\uparrow\uparrow\downarrow} \\ &= 0 \quad (\text{B.9}) \end{aligned}$$

where we have used $z^2 = 1$.

Appendix C: Schwinger Boson Mean Field Theory Calculations

As mentioned in section VI, optimization of multiple parameters occurring in the Schwinger Boson theory for non uniform systems was quite a challenging task. Hence, for the interested reader, we report the exact values of the parameters obtained from our calculations, so that they may be able to reproduce our results.

The optimal mean field parameters are tabulated in Table V for different lattice sizes. In each column (from top to down) the parameters label inner to outermost most bonds/sites. The Q_{ij} 's alternate in strength across successive bonds consistent with the location of unpaired spins. Similar alternation in the condensate field β_i indicates the variation in the density of dangling spins across shells.

The ground state energy from SBMFT for the 126 site cluster was found to be $\approx -0.533J$. This is lower than the DMRG estimate $-0.39385J$. This can be attributed to the well known fact^{44,48} about the non variational nature of SBMFT energies. This is because of not satisfying the constraints in Eq.(6.3) exactly.

N_s	Q_{ij}^*	λ_i^*	β_i^*	N_s	Q_{ij}^*	λ_i^*	β_i^*
14	0.672	1.639	0	126	-0.568	1.893	0.43
	0.539	2.318	0		-0.622	1.656	0.445
	0.676	0.523	0		-0.579	2.026	0.392
30	0.561	1.921	0	254	-0.622	1.497	0.42
	0.633	1.487	0		-0.55	2.32	0.353
	0.543	2.345	0		-0.677	0.546	0.443
	0.673	0.536	0		-0.631	1.669	0.495
62	0.646	1.72	0	254	-0.56	1.986	0.454
	0.57	1.975	0		-0.622	1.537	0.504
	0.63	1.514	0		-0.571	1.965	0.455
	0.551	2.345	0		-0.622	1.495	0.497
	0.68	0.544	0		-0.55	2.263	0.449
					-0.671	0.563	0.56

Table V: Optimal SBMFT parameters for bond centered clusters of various sizes

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